arXiv:cond-mat/9708184v1 [cond-mat.dis-nn] 22 Aug 1997

# Anisotropic Quantum Transport in Layered High–$T_c$ Cuprates

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## Abstract

A random lattice model with dilute interlayer bonds of density $p$ is proposed to describe the underdoped high–$T_c$ cuprates. We show analytically via an appropriate perturbation expansion and verify independently by numerical scaling of the conductance that for any finite $p$ the states remain extended in all directions, despite the presence of interlayer disorder. However, the obtained electronic transport is highly anisotropic with violent conductance fluctuations occuring in the layering direction, which can be responsible for the experimentally observed metallic "in-plane" and semiconducting "out-of-plane" resistivity of the cuprates.

PACS numbers: 72.15.Rn, 71.30.+h, 74.25.Fy

In recent years there is a great interest in the problem of Anderson localization for anisotropic systems [1–6], in connection to the unusual normal–state transport properties of the layered high–$T_c$ cuprates. The in–plane resistivity for most of these materials exhibits metallic behavior, inreasing linearly with temperature over a wide temperature range, while the out–of–plane resistivity is reminiscent of semiconductors increasing rapidly at low temperatures [7–10]. This contrasting behavior of the parallel and the perpendicular resistivities was observed in $Bi_2Sr_{2-x}La_xCuO_y$ far below $T_c$, down to the lowest experimental temperature [11]. Logarithmic divergencies of the corresponding resistivities accompanied by a nearly constant anisotropy ratio are, instead, observed in the underdoped $La_{2-x}Sr_xCuO_4$ suggesting an unusual three-dimensional ($3D$) insulator.

There is currently no consensus on the explanation of the peculiar *ab*-plane "metallic" and the *c*–axis "semiconducting" transport properties of the cuprates, although it is commonly believed that the anisotropic conductivity is, somehow, related to their layered structure. It is also widely thought that understanding the peculiar *c*–axis transport might have important consequences for the high–$T_c$ superconductivity in the cuprates. In this respect, many theoretical models investigate localization in the presence of structural anisotropy, for example, the Anderson model with diagonal disorder and anisotropic hopping $t$ between the $2D$ planes was recently shown to display very different localization lengths in the parallel and the perpendicular directions but the same critical behavior [6]. Although this is in agreement with the scaling theory of localization for anisotropic systems [12–15] is rather inconsistent with the observed contrasting resistivities of the cuprates, which has often been regarded as evidence for their non–Fermi liquid nature [16].

The intense study of the cuprates did not remove many conflicting discrepancies between theory and experiment so that a proper description of anisotropic disorder is strongly desirable. It must be pointed out that previous disordered site potentials with fixed but different hoppings in the lattice axes imply anisotropy only in the band structure and not in the disorder configurations which remain isotropic. We propose that in order to understand the high-$T_c$ cuprates disorder in the anisotropy must be also incorporated. Anisotropic site

randomness in a form resembling a random superlattice with lateral inhomogeneities gave anisotropic localization if the anisotropy was below a critical value, even for arbitrarily small disorder [5]. However, this approach is not a very suitable description for the cuprates either, since the $CuO_2$ planes are believed to be identical with no superlattice–like disorder in the layering direction. The important contribution to the $c$-axis transport in these materials is expected to arise from electron scattering in the "insulating" layer between the conducting $CuO_2$ layers [7–10]. On the other hand, in almost all high-$T_c$ cuprates doping impurities or oxygen vacancies always occupy the insulating layers between the conducting "pure" $CuO_2$ planes which leads to interlayer disorder.

Having the above considerations in mind we propose a very simple $3D$ model with anisotropy both in the band structure and the disorder configuration. The system consists of perfect parallel lattice planes randomly connected by interplane bonds described by the Hamiltonian

$$H = \sum_{l} \sum_{\langle \mathbf{m},\mathbf{n} \rangle} |l,\mathbf{m}\rangle\langle l,\mathbf{n}| + \sum_{l,\mathbf{m}} t\rho_{l,\mathbf{m}}(|l,\mathbf{m}\rangle\langle l+1,\mathbf{m}| + \text{H. c.}), \tag{1}$$

where $\mathbf{m}$, $\mathbf{n}$ are the site indices in every plane and $l$ the plane index. The first term in Eq. (1) describes nearest-neighbor intraplane hopping of unit strength which sets the energy unit. The second term denotes binary alloy–type of disorder which amounts to interplane hoppings $t$ placed at the random planar positions $\mathbf{m}$, implying $100(1-p)\%$ broken longitudinal bonds which inhibit particle migration in the layering direction. The random variable $\rho_{l,\mathbf{m}}$ obeys the distribution

$$P(\rho) = (1-p)\delta(\rho) + p\delta(1-\rho),$$

where $p$ is the perpendicular bond density. As a first step towards the explanation of the normal–state properties of these materials diagonal disorder is ignored so that the in–plane lattices are assumed perfect and the disorder represented by $p$ is due to impurities or oxygen vacancies in the insulating layer among the $2D$ planes. The electrons propagating in this system encounter anisotropy in the disorder due to the random interplane links, in addition to band structure anisotropy due to $t$ being different than one.

A convenient representation for $H$ is the Bloch-Wannier basis

$$|\mathbf{k}_\parallel, l\rangle = \frac{1}{\sqrt{N_\parallel}} \sum_{\mathbf{m}} e^{i\mathbf{k}_\parallel \cdot \mathbf{m}} |l, \mathbf{m}\rangle, \tag{2}$$

where $\mathbf{k}_\parallel$ is the parallel momentum which characterizes the periodic plane states and $N_\parallel$ the number of sites in every plane. In order to investigate the possibility of localization across the planes we define the Green function

$$G_\parallel(\mathbf{k}_\parallel, l; \mathbf{k}'_\parallel, l'; t) \equiv -i\theta(t)\langle [c_{\mathbf{k}_\parallel, l}(t), c^\dagger_{\mathbf{k}'_\parallel, l'}(0)]_+ \rangle, \tag{3}$$

whose diagonal elements give the probability for finding an electron on layer $l$ at time $t$ with momentum $\mathbf{k}_\parallel$, if initially ($t = 0$) was on the same layer with the same momentum. The Fourier transform of the diagonal Green function reads

$$G_\parallel(\mathbf{k}_\parallel, l; \mathbf{k}_\parallel, l; E) = \frac{1}{E - \Sigma_\parallel(\mathbf{k}_\parallel, l, E)} \tag{4}$$

with the self-energy $\Sigma_\parallel$ written as [17,18]

$$\Sigma_\parallel(\mathbf{k}_\parallel, l, E) = \epsilon_\parallel(\mathbf{k}_\parallel) + \sum_{n=1}^{\infty} \sum_j T_j^{(n)}, \tag{5}$$

where the $n$-th order term is a sum over all paths $j$ starting and ending on the initial layer state with

$$T_j^{(n)} = V(\mathbf{k}_\parallel, l; \mathbf{k}_{\parallel_1}, l_1) \prod_{i=1}^{n} \frac{V(\mathbf{k}_{\parallel_i}, l_i; \mathbf{k}_{\parallel_{i+1}}, l_{i+1})}{E - \epsilon_\parallel(\mathbf{k}_{\parallel_i})} \tag{6}$$

and $\mathbf{k}_{\parallel_{n+1}} = \mathbf{k}_\parallel, l_{n+1} = l$. The perfect plane Bloch states characterized by $\mathbf{k}_{\parallel_i}$ have energy

$$\epsilon_\parallel(\mathbf{k}_{\parallel_i}) = 2\cos(k_{x_i}) + 2\cos(k_{y_i}), \tag{7}$$

while the interplane hopping which appears in Eq. (6) in the plane-diagonal representation takes the form

$$V(\mathbf{k}_{\parallel_i}, l_i; \mathbf{k}_{\parallel_{i+1}}, l_{i+1}) = \frac{t}{N_\parallel} \sum_{\mathbf{m}} e^{i(\mathbf{k}_{\parallel_i} - \mathbf{k}_{\parallel_{i+1}}) \cdot \mathbf{m}} \delta_{l_{i+1}, l_i \pm 1}, \tag{8}$$

with the sum over $\mathbf{m}$ denoting only the layer sites having bonds present to the nearest neighbor layers. It is seen from Eq. (8) that the diagonal in momentum ($\mathbf{k}_{\parallel_i} = \mathbf{k}_{\parallel_{i+1}}$) matrix

elements are exactly $pt$ and for a given order $n$ if $E$ lies within the $2D$ band $\epsilon_{\|}(\mathbf{k}_{\|_i})$ the most divergent term of Eq. (5) comes from the path which has intermediate states $|\mathbf{k}_{\|_i}, l_i\rangle$ with $\epsilon_{\|}(\mathbf{k}_{\|_i}) = E$. The corresponding term is $(pt/(E - \epsilon_{\|}(\mathbf{k}_{\|_i}))^n$ and nearest neighbor plane states with the same $\mathbf{k}_{\|}$ are predominantly connected. It can be also seen that momentum scattering is always accompanied by interlayer hopping since a change of $\mathbf{k}_{\|}$ always leads to a change of layer. Therefore, $H$ can be tranformed into an "undisturbed" term $H_0$ which represents a perfect anisotropic $3D$ lattice with on-plane (interlayer) hopping 1 ($pt$), plus the rest which forms a "random" $H_1$ hamiltonian part with matrix elements

$$v(\mathbf{k}, \mathbf{k}') = \begin{cases} \frac{t(e^{ik_z} + e^{-ik'_z})}{N} \sum_l \sum_{\mathbf{m}_l} e^{i(\mathbf{k}_{\|} - \mathbf{k}'_{\|}) \cdot \mathbf{m}_l + i(k_z - k'_z)l}, \text{ for } \mathbf{k}_{\|} \neq \mathbf{k}'_{\|}, \\ 0, \text{ for } \mathbf{k}_{\|} = \mathbf{k}'_{\|}, \end{cases} \tag{9}$$

expressed in the $H_0$-diagonal basis $|\mathbf{k}\rangle = |\mathbf{k}_{\|}, k_z\rangle$, where $N$ is the total number of lattice sites, $l$ the layer index, $k_z$ the perpendicular momentum and the sum over $\mathbf{m}_l$ runs over sites which are connected to nearest neighbor planes by interplane bonds. In the adopted basis $H_1$ has only off-diagonal matrix elements in the momentum $\mathbf{k}_{\|}$ between planes since the diagonal elements were already included in $H_0$.

In order to determine the properties for the eigenstates of $H_0$ characterized by $\mathbf{k}$, with corresponding eigenvalues $\epsilon(\mathbf{k})$, we can expand the corresponding self-energy $\Sigma(\mathbf{k}, E)$ as in Eq. (5) via the expansion parameter

$$T(E, \mathbf{k}') = \sum_{\mathbf{k}''} \frac{v(\mathbf{k}', \mathbf{k}'')}{E - \epsilon(\mathbf{k}'')} \tag{10}$$

and if Eq. (9) is substituded into Eq. (10)

$$T(E, \mathbf{k}') = \sum_{\mathbf{k}''} \sum_l \sum_{\mathbf{m}_l} \frac{t(e^{ik'_z} + e^{-ik''_z}) e^{i(\mathbf{k}'_{\|} - \mathbf{k}''_{\|}) \cdot \mathbf{m}_l + i(k'_z - k''_z)l}}{N[E - \epsilon(\mathbf{k}'')]} \tag{11}$$

evidently vanishes on average taken over a large number of configurations, since all the on-plane site positions will be exhausted for the present interplane bonds by the additional sum for the average which leads to cancellations in Eq. (11) from Bloch theorem. A typical $T$ for a given random configuration fluctuates around zero with a variance $\sigma^2_{\text{sum}} \sim Q\sigma^2$, where $\sigma^2$ is the variance of a single term and $Q$ the total number of terms in the sum. According to the

denominator $E-\epsilon(\mathbf{k}'')$ the most important contribution comes from states with momenta on an equal-energy surface in the $\mathbf{k}$-space whose number is of the order of $N_{\parallel}=L^2$. The total number of present interplane bonds is $pL^3$ which gives $Q\sim pL^5$, so that for a given configuration the sum is $\sim\sqrt{p}L^{\frac{5}{2}}$. Finally, by including the normalization factor $N=L^3$ in the denominator $T(E,\mathbf{k}')\sim\sqrt{p}L^{-\frac{1}{2}}$ which guarantees rapid convergence of the self-energy in $\mathbf{k}$-space to

$$\Sigma(\mathbf{k},E)\simeq\epsilon(\mathbf{k})+\sum_{\mathbf{k}'}\frac{|v(\mathbf{k},\mathbf{k}')|^2}{E-\epsilon(\mathbf{k}')}. \tag{12}$$

The configuration average $\langle Im\sum_{\mathbf{k}'}\frac{|v(\mathbf{k},\mathbf{k}')|^2}{E-\epsilon(\mathbf{k}')-i0^+}\rangle$ is also computed as a function of $p$ and the obtained semicircular form can be fitted by $\rho(E)t^2p(1-p)$, with $E$ within the $H_0$ band with $\rho(E)$ the density of states. This allows to estimate the lifetime of states $\tau\sim\frac{1}{\rho(E)t^2p(1-p)}$ and the corresponding mean free paths

$$\lambda_{\parallel}=\frac{\tau u_{\parallel}^2}{u}\simeq\frac{1}{\rho(E)t^2p(1-p)\sqrt{2+p^2t^2}}, \tag{13}$$

$$\lambda_{\perp}=\frac{\tau u_{\perp}^2}{u}\simeq\frac{p}{\rho(E)(1-p)\sqrt{2+p^2t^2}}, \tag{14}$$

by taking into account the Fermi velocites $u_{\parallel(\perp)}$. It can be seen that for small-$p$ the parallel (perpendicular) mean free path is proportional to $1/p$ ($p$) so that the interlayer disorder affects more the perpendicular transport although cannot localize the states even in this direction.

The predicted extended nature of the wave functions is independently verified by numerical scaling of the conductance in finite systems. The parallel (perpendicular) conductance $G_{\parallel(\perp)}(L)$ as a function of the linear size $L$ is obtained for a cubic system at the Fermi energy $E$ from the multichannel Landauer–Buttiker formula [19–21]

$$G_{\parallel(\perp)}(L)=(e^2/h)\mathrm{Tr}(T_{\parallel(\perp)}^{+}T_{\parallel(\perp)}), \tag{15}$$

where $T_{\parallel(\perp)}$ is the transmission matrix for electronic propagation along the parallel (perpendicular) direction which can be obtained by transfer matrix techniques. The matrix $T_{\perp}$

turns out to be singular due to the presence of zeros for the missing bonds. This difficulty can be dealt with succesfully if we introduce hard-wall boundary conditions in the parallel directions and assign a unit incident wave amplitude for one channel, with zero for the rest, at a time. The recursion relations for the corresponding wave function coefficients are easily established along the parallel direction while along the difficult perpendicular direction the assignment made for the incident waves is used as a boundary condition. This is a convenient method which allows to consider propagation in the difficult layering direction by a transfer matrix product in the easy parallel direction since the $L^2$ equations for the the unknown coefficients can be solved. The absence of missing bonds in the parallel direction makes the recursion relations no longer singular and $T_\perp$ can be obtained for the output channels, for every assignement made for the input channels. In the calculations we have taken averages over up to a 5000 random configurations in each case to suppress fluctuations.

In Figure 1 we show the scaling behavior of the dimensionless conductance $g_{\parallel(\perp)}(L) = G_{\parallel(\perp)}(L)/(e^2/h)$ with anisotropic interplane coupling $t = 0.3$ for various bond densities $p$. The parallel conductance increases ballistically ($\sim L^2$) for small $L$ and linearly for higher $L$. In the large size ($L \to \infty$) limit the scaling function $\beta(L) = d\ln g/d\ln L$ is positive for $g_{\parallel(\perp)}$, which implies extended states in both directions for any $p$ in agreement with our analytical results. However, the transport behavior found is essentially different in the two directions. In Fig. 2 we show the energy dependence of the conductance for $p = 0.5$ and $t = 0.3$ where the ratio of the conductances is close to the estimate $g_\parallel/g_\perp \simeq (t_\parallel/t_\perp)^2$ [6] for $t_\parallel = 1$ and $t_\perp = pt = 0.15$. Another key finding from Fig. 2 is a rather smooth $g_\parallel(E)$ while $g_\perp(E)$ displays violent oscillations as a function of $E$. The dips in $g_\perp(E)$ can be ragarded as "minigaps" which might have an effect similar to a semiconductor leading to insulating kind of behavior for the out-of-plane conductivity when the Fermmi energy is varied.

We argue that the proposed model is closely related to high–$T_c$ cuprates. As the temperature increases the inelastic scattering in these materials due to phonons, spin waves or other excitations within the $CuO_2$ layers can cause a decrease of the characteristic inelastic scattering lengths $l_{in}$. If the temperature is so high that $l_{in}$ becomes smaller than the

mean free path caused from the "random" Hamiltonian $H_1$ the transverse conductivity becomes perfectly metallic. Experiments for $Bi_2Sr_2CaCu_2O_8$ and underdoped $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+x}$ give out–of–plane resistivity which has a semiconductor–like temperature dependence at low temperatures and a linear–in–$T$ behavior at high temperatures with characteristic crossover temperature $T^*$ between the two regimes, which decreases by increasing doping in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ [7–10]. We notice that if we relate the bond density $p$ with the doping density of the high-$T_c$ materials the obtained $p$-dependence of the perpendicular mean free path can be used to explain qualitatively the reported experimental behavior. It must be pointed out that the relation between the cuprate doping density and the bond density $p$ is very natural, since an increase in the number of the doping impurities or the oxygen atoms in the layer between two $CuO_2$ planes increases the number of hopping paths between the two planes. As $T^*$ decreases further below the superconducting transition temperature $T_c$ the out–of–plane normal–state resistivity also becomes metallic, which has recently been observed in high–quality single crystals of $YBA_2Cu_3O_7$ and other high–$T_c$ cuprates [22] corresponding to the absence of disorder ($p \approx 1$ in the proposed model) with almost infinite perpendicular mean free path. This effect can be observed only in the perpendicular direction since the parallel mean free path is always much longer and the inelasting scattering more dominant in ths direction.

In summary, we have introduced a simple layered lattice model for high-$T_c$ cuprates based on the fact that these materials consist of pure $CuO_2$ planes while doping impurities or oxygen vacancies occupy randomly the interplane hopping paths. We introduce anisotropic disorder described by the interplane bond density $p$, in addition to the usual anisotropic band structure expressed via the interplane hopping strength $t$. In the absence of diagonal disorder we show extended states in both directions but the obtained mean free path and the conductance in the perpendicular direction is much smaller than the parallel one. Moreover, the perpendicular conductance fluctuates strongly as a function of energy, which might lead to an insulator-like temperature dependence of the conductivity in this direction. To conclude, we have demonstrated anisotropic transport which can account for experimental

facts of high-$T_c$ cuprates. More work is needed in order to understand the corresponding metal-insulator transition of layering materials also in the presence of diagonal disorder and/or a homogenous magnetic field.

**Acknowledgments**

This work was supported in part by a TMR grant and also a ΠΕΝΕΔ Research Grant of the Greek Secretariat of Science and Technology.

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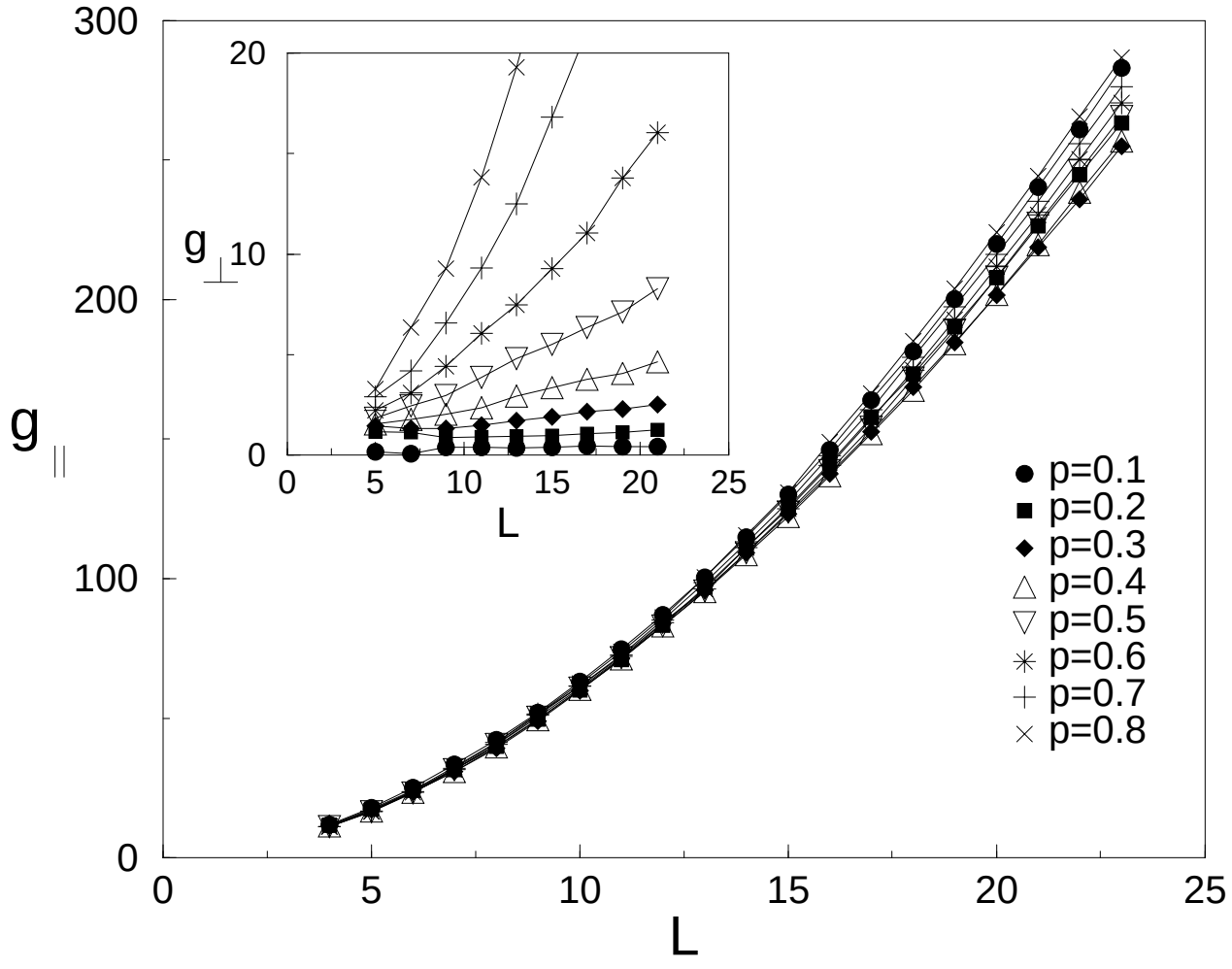
## FIGURES

**FIG.1**. The $g_{\|}$ as a function of the linear system size $L$ for a cubic system of parallel planes with randomly placed interplane bonds of density $p$ and strength $t = 0.3$. In the inset $g_{\perp}$ is shown for the same system.

**FIG.2**. (**a**) The energy-dependent $g_{\|}$ for a layered system with $L = 10, 15$ and $t = 0.3$, $p = 0.5$. (**b**) A much smaller $g_{\perp}$ is shown which exhibits violent oscillations as a function of energy.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200
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0
5
10
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20
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L
g||
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L
g⊥
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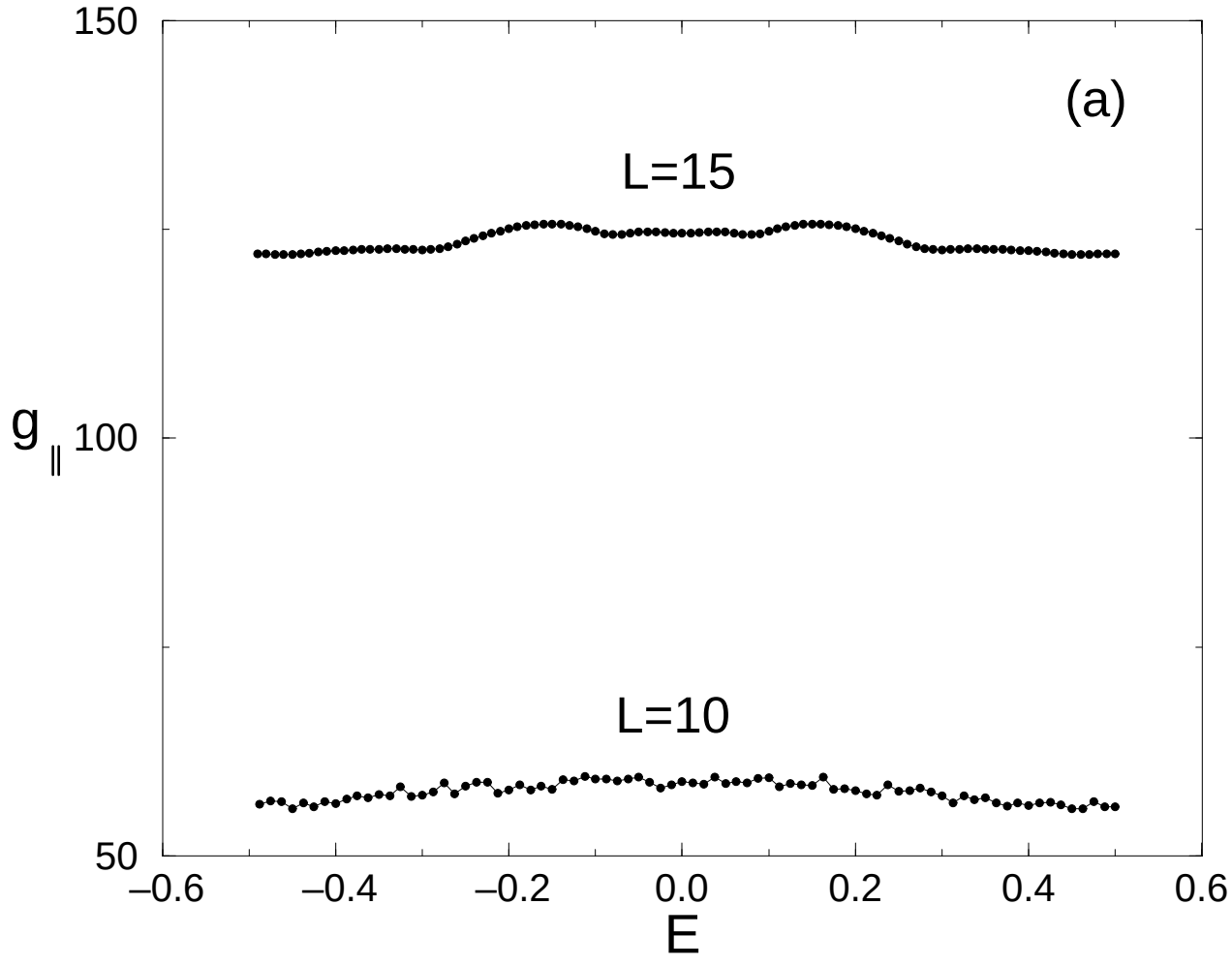
p=0.4
p=0.5
p=0.6
p=0.7
p=0.8


150
100
50
(a)
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L=10
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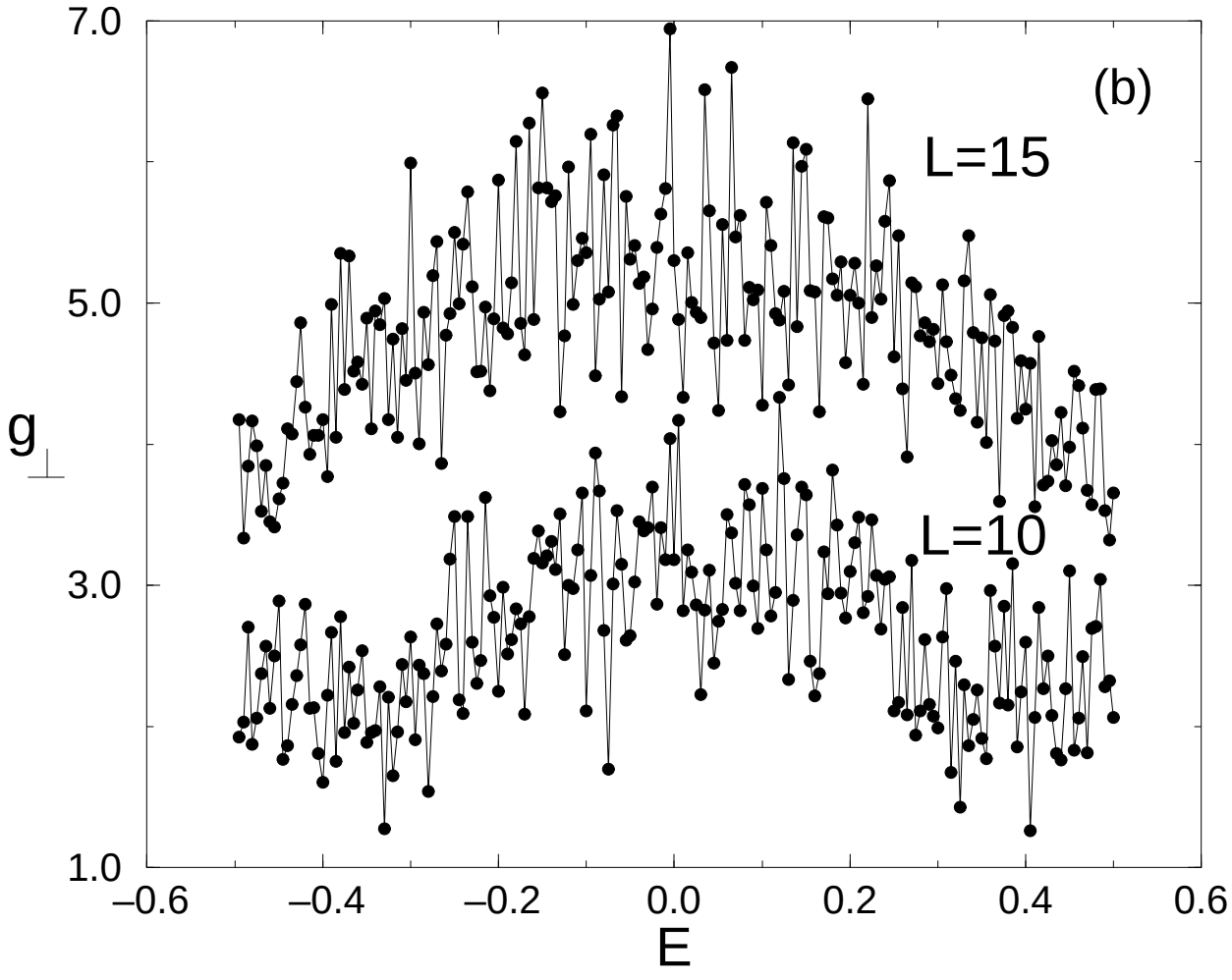
–0.2
0.0
0.2
0.4
0.6
E


7.0
5.0
3.0
1.0
g⊥
(b)
L=15
L=10
–0.6
–0.4
–0.2
0.0
0.2
0.4
0.6
E